

10/542,003

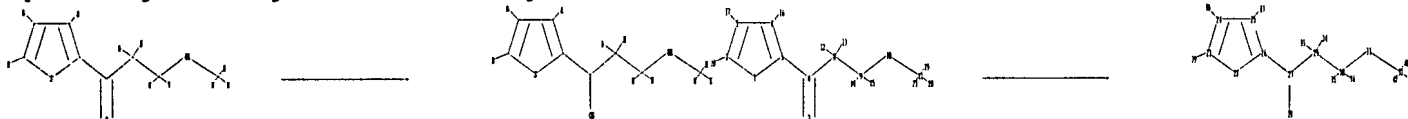
Search w/ enzyme

*
* CASREACT now has more than 10 million reactions *
*

Some CASREACT records are derived from the ZIC/VINITI database (1974-1991) provided by InfoChem, INPI data prior to 1986, and Biotransformations database compiled under the direction of Professor Dr. Klaus Kieslich.

This file contains CAS Registry Numbers for easy and accurate substance identification.

=>
Uploading C:\Program Files\Stnexp\Queries\Karen3.str



chain nodes :
6 7 8 9 10 11 12 13 14 15 16 17 18 19 20 21 27 28 29 30 31 32 33
34 35 36 37 38 39 40 41 42
ring nodes :
1 2 3 4 5 22 23 24 25 26
chain bonds :
2-18 3-17 4-16 5-6 6-7 6-8 8-9 8-12 8-13 9-10 9-14 9-15 10-11 11-19 11-20
11-21 23-39 24-38 25-37 26-27 27-29 27-28 29-30 29-33 29-34 30-31 30-35 30-36
31-32 32-40 32-41 32-42
ring bonds :
1-2 1-5 2-3 3-4 4-5 22-23 22-26 23-24 24-25 25-26
exact/norm bonds :
1-2 1-5 2-3 3-4 4-5 9-10 10-11 22-23 22-26 23-24 24-25 25-26 27-28 30-31
31-32
exact bonds :
2-18 3-17 4-16 5-6 6-7 6-8 8-9 8-12 8-13 9-14 9-15 11-19 11-20 11-21 23-39
24-38 25-37 26-27 27-29 29-30 29-33 29-34 30-35 30-36 32-40 32-41 32-42

Match level :
1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:CLASS 7:CLASS 8:CLASS 9:CLASS 10:CLASS
11:CLASS 12:CLASS 13:CLASS 14:CLASS 15:CLASS 16:CLASS 17:CLASS 18:CLASS 19:CLASS
20:CLASS 21:CLASS 22:Atom 23:Atom 24:Atom 25:Atom 26:Atom 27:CLASS 28:CLASS
29:CLASS 30:CLASS 31:CLASS 32:CLASS 33:CLASS 34:CLASS 35:CLASS 36:CLASS 37:CLASS
38:CLASS 39:CLASS 40:CLASS 41:CLASS 42:CLASS

L4 STRUCTURE UPLOADED

=> s 14 ful
FULL SEARCH INITIATED 14:33:18 FILE 'CASREACT'
SCREENING COMPLETE - 1512 REACTIONS TO VERIFY FROM 270 DOCUMENTS

100.0% DONE 1512 VERIFIED 22 HIT RXNS 8 DOCS
SEARCH TIME: 00.00.01

L5 8 SEA SSS FUL L4 (22 REACTIONS)

10/5/2006

10/542,003

=> s l5 and (enzyme or microbial or dehydrogenase or enantioselective or catalyst)

10805 ENZYME

2788 MICROBIAL

1375 DEHYDROGENASE

12257 ENANTIOSELECTIVE

81437 CATALYST

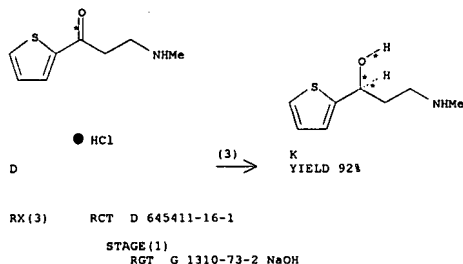
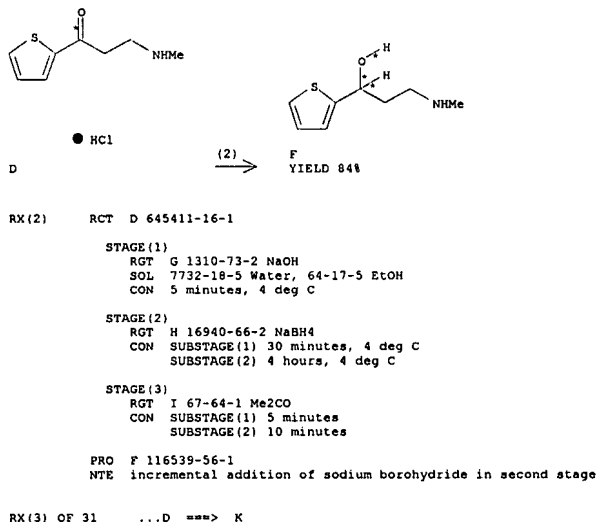
L6 6 L5 AND (ENZYME OR MICROBIAL OR DEHYDROGENASE OR ENANTIOSELECTIVE
OR CATALYST)

=> d ibib abs hit 1-6

L6 ANSWER 1 OF 6 CASREACT COPYRIGHT 2006 ACS on STN
 ACCESSION NUMBER: 143:248273 CASREACT
 TITLE: Preparation of enantiomerically pure
 1-substituted-3-amino alcohols
 INVENTOR(S): Michel, Dominique
 PATENT ASSIGNEE(S): Lonza A.-G., Switz.
 SOURCE: Eur. Pat. Appl., 14 pp.
 CODEN: EPXXDW
 DOCUMENT TYPE: Patent
 LANGUAGE: English
 FAMILY ACC. NUM. COUNT: 2
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
EP 1566393	A1	20050824	EP 2004-3809	20040219
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, SK				
WO 2005080370	A1	20050901	WO 2005-EP1781	20050221
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW				
RW: BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG				
PRIORITY APPLN. INFO.: EP 2004-3809 20040219 EP 2004-10043 20040428				
OTHER SOURCE(S): MARPAT 143:248273				
AB Provided is a process for the preparation of enantiomerically pure 1-substituted-3-amino alcs. (R)- or (S)-HOCH(R1)CH2CH2NHR2 (R1 = 2-thienyl, 2-furanyl, Ph, substituted 2-thienyl, substituted 2-furanyl, substituted Ph; R2 = C1-C4-alkyl, Ph, substituted C1-C4-alkyl, substituted Ph), particularly (S)-(-)- and (R)-(+)-3-N-methylamino-1-(2-thienyl)-1-propanol, by asym. hydrogenating salts of R1COCH2CH2NHR2 using Rh and an asym. ligand.				
REFERENCE COUNT: 10 THERE ARE 10 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT				
RX(2) OF 31 ...D ==> F				

L6 ANSWER 1 OF 6 CASREACT COPYRIGHT 2006 ACS on STN (Continued)



L6 ANSWER 1 OF 6 CASREACT COPYRIGHT 2006 ACS on STN (Continued)

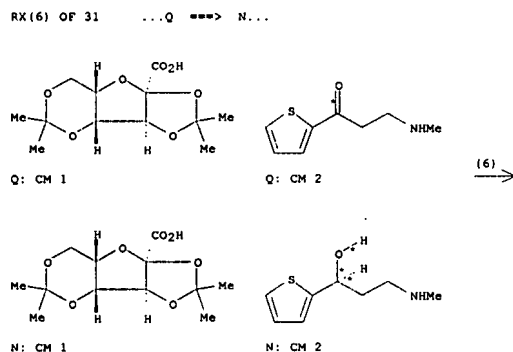
SOL 67-56-1 MeOH
 CON room temperature

STAGE(2)
 SOL 67-56-1 MeOH
 CON SUBSTAGE(1) room temperature
 SUBSTAGE(2) room temperature -> 50 deg C

STAGE(3)
 RGT L 1333-74-0 H2
 CON SUBSTAGE(1) 50 deg C, 30 bar
 SUBSTAGE(2) 5 hours, 50 deg C
 SUBSTAGE(3) 50 deg C -> room temperature

PRO K 116539-55-0
 NTE [Rh((R,R,S,S)-Me-Duphos)]BF4 used as catalyst stage 2, stereoselective, autoclave used, high pressure in last stage, ee = 97%, optimized on catalyst

RX(6) OF 31 ...Q ==> N...



RX(6) RCT Q 863094-06-8

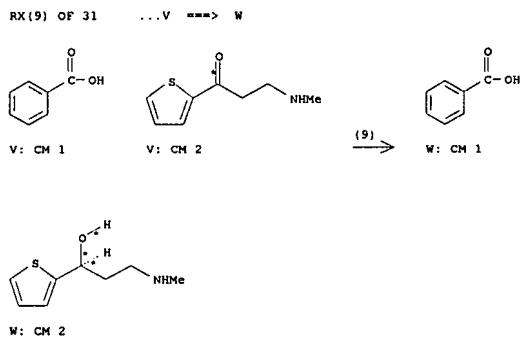
STAGE(1)
 SOL 67-56-1 MeOH
 CON SUBSTAGE(1) room temperature
 SUBSTAGE(2) room temperature
 SUBSTAGE(3) room temperature -> 50 deg C

STAGE(2)
 RGT L 1333-74-0 H2
 CON SUBSTAGE(1) 50 deg C, 30 bar
 SUBSTAGE(2) 5 hours, 50 deg C
 SUBSTAGE(3) 50 deg C -> room temperature

PRO N 569687-76-9

L6 ANSWER 1 OF 6 CASREACT COPYRIGHT 2006 ACS on STN (Continued)

NTE [Rh((R,R,S,S)-tangphos)(norbornadiene)]BF4 used as catalyst stage 1, stereoselective, high pressure in last stage, autoclave used, ee = 95%, conversion is 100%



RX(9) RCT V 863094-15-9

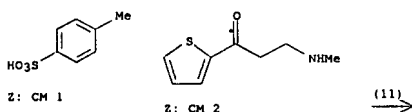
STAGE(1)
 CAT 205064-10-4 Rhodium(1+), [(1,2,5,6-η)-1,5-cyclooctadiene][(2S,2'S,5S,5'S)-1,1'-(1,2-phenylene)bis(2,5-dimethylphospholane-κP)]-, tetrafluoroborate(1-)
 SOL 67-56-1 MeOH
 CON SUBSTAGE(1) room temperature
 SUBSTAGE(2) room temperature -> 50 deg C

STAGE(2)
 RGT L 1333-74-0 H2
 CON SUBSTAGE(1) 50 deg C, 30 bar
 SUBSTAGE(2) 5 hours, 50 deg C
 SUBSTAGE(3) 50 deg C -> room temperature

PRO W 863094-19-3
 NTE stereoselective, high pressure in last stage, autoclave used, ee = 96.7%, conversion is 99%

RX(11) OF 31 ...Z ==> AA

L6 ANSWER 1 OF 6 CASREACT COPYRIGHT 2006 ACS on STN (Continued)



RX(11) RCT Z 863094-23-9

STAGE(1)

CAT 205064-10-4 Rhodium(I+), [(1,2,5,6-η)-1,5-cyclooctadiene][(2S,2'S,5S,5'S)-1,1'-(1,2-phenylene)bis[2,5-dimethylphospholane-κP]]-, tetrafluoroborate(1-)

SOL 67-56-1 MeOH

CON SUBSTAGE(1) room temperature

SUBSTAGE(2) room temperature -> 50 deg C

STAGE(2)

RGT L 1333-74-0 H2

CON SUBSTAGE(1) 50 deg C, 30 bar

SUBSTAGE(2) 5 hours, 50 deg C

SUBSTAGE(3) 50 deg C -> room temperature

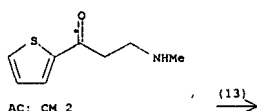
PRO AA 863094-27-3

NTE stereoselective, high pressure in last stage, autoclave used, ee = 90%, conversion is 5%

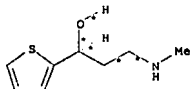
RX(13) OF 31 ...AC ==> AD

HO₂C-(CH₂)₁₀-Me

AC: CM 1



L6 ANSWER 1 OF 6 CASREACT COPYRIGHT 2006 ACS on STN (Continued)



YIELD 92%

RX(1) RCT A 88-15-3, B 50-00-0, C 593-51-1

PRO D 645411-16-1

SOL 64-17-5 EtOH

CON SUBSTAGE(1) 9 hours, 120 - 130 deg C

SUBSTAGE(2) 130 deg C -> 20 deg C

NTE paraformaldehyde used, autoclave used

RX(3) RCT D 645411-16-1

STAGE(1)

RGT G 1310-73-2 NaOH

SOL 67-56-1 MeOH

CON room temperature

STAGE(2)

SOL 67-56-1 MeOH

CON SUBSTAGE(1) room temperature

SUBSTAGE(2) room temperature -> 50 deg C

STAGE(3)

RGT L 1333-74-0 H2

CON SUBSTAGE(1) 50 deg C, 30 bar

SUBSTAGE(2) 5 hours, 50 deg C

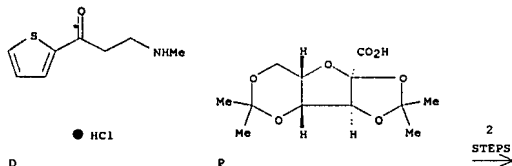
SUBSTAGE(3) 50 deg C -> room temperature

PRO K 116539-55-0

NTE [Rh((S,S)-Me-Duphos)]BF₄ used as catalyst stage 2, stereoselective, autoclave used, high pressure in last stage, ee = 97%, optimized on catalyst

RX(21) OF 31 COMPOSED OF RX(5), RX(6)

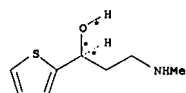
RX(21) D + P ==> N



L6 ANSWER 1 OF 6 CASREACT COPYRIGHT 2006 ACS on STN (Continued)

HO₂C-(CH₂)₁₀-Me

AD: CM 1



AD: CM 2

RX(13) RCT AC 863094-31-9

STAGE(1)

SOL 67-56-1 MeOH

CON SUBSTAGE(1) room temperature

SUBSTAGE(2) room temperature -> 50 deg C

STAGE(2)

RGT L 1333-74-0 H2

CON SUBSTAGE(1) 50 deg C, 30 bar

SUBSTAGE(2) 5 hours, 50 deg C

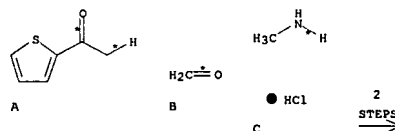
SUBSTAGE(3) 50 deg C -> room temperature

PRO AD 863094-35-3

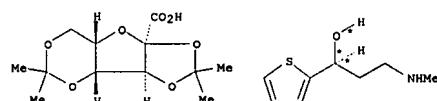
NTE stereoselective, high pressure in last stage, autoclave used, ee = 93.6%, conversion is 100%

RX(15) OF 31 COMPOSED OF RX(1), RX(3)

RX(15) A + B + C ==> K



L6 ANSWER 1 OF 6 CASREACT COPYRIGHT 2006 ACS on STN (Continued)



RX(5) RCT D 645411-16-1

STAGE(1)

RGT G 1310-73-2 NaOH

SOL 7732-18-5 Water, 1634-04-4 t-BuOMe

CON SUBSTAGE(1) room temperature -> 0 deg C

SUBSTAGE(2) 15 minutes, 0 deg C

SUBSTAGE(3) 10 minutes, 0 deg C

STAGE(2)

RCT P 18467-77-1

SOL 1634-04-4 t-BuOMe

CON room temperature

PRO Q 863094-06-8

NTE scalable

RX(6) RCT Q 863094-06-8

STAGE(1)

SOL 67-56-1 MeOH

CON SUBSTAGE(1) room temperature

SUBSTAGE(2) room temperature

SUBSTAGE(3) room temperature -> 50 deg C

STAGE(2)

RGT L 1333-74-0 H2

CON SUBSTAGE(1) 50 deg C, 30 bar

SUBSTAGE(2) 5 hours, 50 deg C

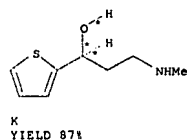
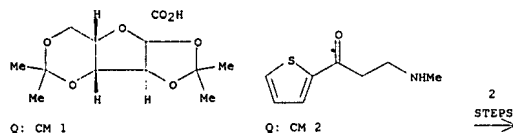
SUBSTAGE(3) 50 deg C -> room temperature

PRO N 569687-76-9

NTE [Rh((R,R,S,S)-tangphos)(norbornadiene)]BF₄ used as catalyst stage 1, stereoselective, high pressure in last stage, autoclave used, ee = 95%, conversion is 100%

RX(22) OF 31 COMPOSED OF RX(6), RX(4)

RX(22) Q ==> K



RX(6) RCT Q 863094-06-8

STAGE(1)
 SOL 67-56-1 MeOH
 CON SUBSTAGE(1) room temperature
 SUBSTAGE(2) room temperature
 SUBSTAGE(3) room temperature -> 50 deg C

STAGE(2)
 RGT L 1333-74-0 H2
 CON SUBSTAGE(1) 50 deg C, 30 bar
 SUBSTAGE(2) 5 hours, 50 deg C
 SUBSTAGE(3) 50 deg C -> room temperature

PRO N 569687-76-9
 NTE [Rh]((R,R,S,S)-tandphos)(norbornadiene)]BF4 used as catalyst stage 1, stereoselective, high pressure in last stage, autoclave used, ee = 95%, conversion is 100%

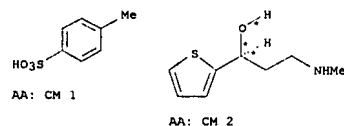
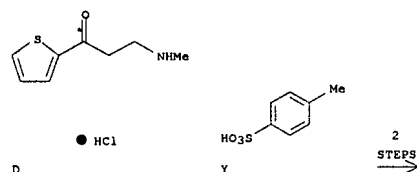
RX(4) RCT N 569687-76-9
 RGT G 1310-73-2 NaOH
 PRO K 116539-55-0
 SOL 7732-18-5 Water, 75-09-2 CH2Cl2
 CON SUBSTAGE(1) room temperature
 SUBSTAGE(2) 15 minutes, room temperature
 NTE incremental addition of reactant

RX(23) OF 31 COMPOSED OF RX(8), RX(9)
 RX(23) D + U ==> W

L6 ANSWER 1 OF 6 CASREACT COPYRIGHT 2006 ACS on STN (Continued)
 SUBSTAGE(3) 50 deg C -> room temperature

PRO W 863094-19-3
 NTE stereoselective, high pressure in last stage, autoclave used, ee = 96.7%, conversion is 99%

RX(24) OF 31 COMPOSED OF RX(10), RX(11)
 RX(24) D + Y ==> AA



RX(10) RCT D 645411-16-1

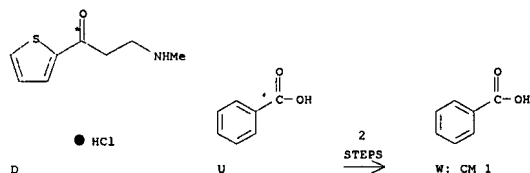
STAGE(1)
 RGT G 1310-73-2 NaOH
 SOL 7732-18-5 Water, 1634-04-4 t-BuOMe
 CON SUBSTAGE(1) room temperature -> 10 deg C
 SUBSTAGE(2) 5 - 10 deg C
 SUBSTAGE(3) 15 minutes, 5 - 10 deg C

STAGE(2)
 RCT Y 104-15-4
 SOL 1634-04-4 t-BuOMe
 CON 15 minutes, <10 deg C

PRO Z 863094-23-9

RX(11) RCT Z 863094-23-9

STAGE(1)
 CAT 205064-10-4 Rhodium(1+), [(1,2,5,6-η)-1,5-cyclooctadiene][(2S,2'S,5S,5'S)-1,1'-(1,2-phenylene)bis[2,5-dimethylphospholane-κP]]-, tetrafluoroborate(1-)
 SOL 67-56-1 MeOH
 CON SUBSTAGE(1) room temperature



W: CM 2

RX(8) RCT D 645411-16-1

STAGE(1)
 RGT G 1310-73-2 NaOH
 SOL 7732-18-5 Water, 1634-04-4 t-BuOMe
 CON SUBSTAGE(1) room temperature -> 10 deg C
 SUBSTAGE(2) 5 - 10 deg C
 SUBSTAGE(3) 15 minutes, 5 - 10 deg C

STAGE(2)
 RCT U 65-85-0
 SOL 1634-04-4 t-BuOMe
 CON 15 minutes, <10 deg C

PRO V 863094-15-9

RX(9) RCT V 863094-15-9

STAGE(1)
 CAT 205064-10-4 Rhodium(1+), [(1,2,5,6-η)-1,5-cyclooctadiene][(2S,2'S,5S,5'S)-1,1'-(1,2-phenylene)bis[2,5-dimethylphospholane-κP]]-, tetrafluoroborate(1-)
 SOL 67-56-1 MeOH
 CON SUBSTAGE(1) room temperature
 SUBSTAGE(2) room temperature -> 50 deg C

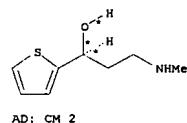
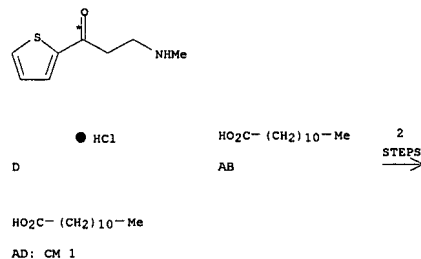
STAGE(2)
 RGT L 1333-74-0 H2
 CON SUBSTAGE(1) 50 deg C, 30 bar
 SUBSTAGE(2) 5 hours, 50 deg C

L6 ANSWER 1 OF 6 CASREACT COPYRIGHT 2006 ACS on STN (Continued)
 SUBSTAGE(2) room temperature -> 50 deg C

STAGE(2)
 RGT L 1333-74-0 H2
 CON SUBSTAGE(1) 50 deg C, 30 bar
 SUBSTAGE(2) 5 hours, 50 deg C
 SUBSTAGE(3) 50 deg C -> room temperature

PRO AA 863094-27-3
 NTE stereoselective, high pressure in last stage, autoclave used, ee = 90%, conversion is 5%

RX(25) OF 31 COMPOSED OF RX(12), RX(13)
 RX(25) D + AB ==> AD



RX(12) RCT D 645411-16-1

STAGE(1)
 RGT G 1310-73-2 NaOH
 SOL 7732-18-5 Water, 1634-04-4 t-BuOMe
 CON SUBSTAGE(1) room temperature -> 10 deg C
 SUBSTAGE(2) 5 - 10 deg C
 SUBSTAGE(3) 15 minutes, 5 - 10 deg C

STAGE(2)
 RCT AB 143-07-7
 SOL 1634-04-4 t-BuOMe

L6 ANSWER 1 OF 6 CASREACT COPYRIGHT 2006 ACS on STN (Continued)

CON SUBSTAGE(1) 15 minutes, <10 deg C
SUBSTAGE(2) 1 hour

PRO AC 863094-31-9

RX(13) RCT AC 863094-31-9

STAGE(1)

SOL 67-56-1 MeOH

CON SUBSTAGE(1) room temperature

SUBSTAGE(2) room temperature -> 50 deg C

STAGE(2)

RGT L 1333-74-0 H2

CON SUBSTAGE(1) 50 deg C, 30 bar

SUBSTAGE(2) 5 hours, 50 deg C

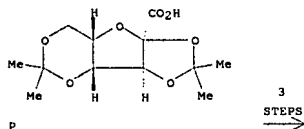
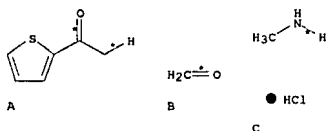
SUBSTAGE(3) 50 deg C -> room temperature

PRO AD 863094-35-3

NTE stereoselective, high pressure in last stage, autoclave used, ee = 93.6%, conversion is 100%

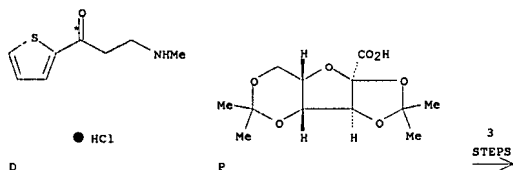
RX(26) OF 31 COMPOSED OF RX(1), RX(5), RX(6)

RX(26) A + B + C + P ==> N



L6 ANSWER 1 OF 6 CASREACT COPYRIGHT 2006 ACS on STN (Continued)

RX(30) D + P ==> K



K
YIELD 87%

RX(5) RCT D 645411-16-1

STAGE(1)

RGT G 1310-73-2 NaOH

SOL 7732-18-5 Water, 1634-04-4 t-BuOMe

CON SUBSTAGE(1) room temperature -> 0 deg C

SUBSTAGE(2) 15 minutes, 0 deg C

SUBSTAGE(3) 10 minutes, 0 deg C

STAGE(2)

RGT P 18467-77-1

SOL 1634-04-4 t-BuOMe

CON room temperature

PRO Q 863094-06-8

NTE scalable

RX(6) RCT Q 863094-06-8

STAGE(1)

SOL 67-56-1 MeOH

CON SUBSTAGE(1) room temperature

SUBSTAGE(2) room temperature

SUBSTAGE(3) room temperature -> 50 deg C

STAGE(2)

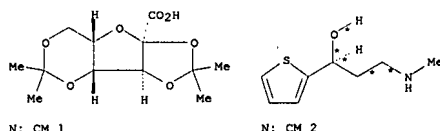
RGT L 1333-74-0 H2

CON SUBSTAGE(1) 50 deg C, 30 bar

SUBSTAGE(2) 5 hours, 50 deg C

SUBSTAGE(3) 50 deg C -> room temperature

L6 ANSWER 1 OF 6 CASREACT COPYRIGHT 2006 ACS on STN (Continued)



RX(1) RCT A 88-15-3, B 50-00-0, C 593-51-1

PRO D 645411-16-1

SOL 64-17-5 EtOH

CON SUBSTAGE(1) 9 hours, 120 - 130 deg C

SUBSTAGE(2) 130 deg C -> 20 deg C

NTE paraformaldehyde used, autoclave used

RX(5) RCT D 645411-16-1

STAGE(1)

RGT G 1310-73-2 NaOH

SOL 7732-18-5 Water, 1634-04-4 t-BuOMe

CON SUBSTAGE(1) room temperature -> 0 deg C

SUBSTAGE(2) 15 minutes, 0 deg C

SUBSTAGE(3) 10 minutes, 0 deg C

STAGE(2)

RGT P 18467-77-1

SOL 1634-04-4 t-BuOMe

CON room temperature

PRO Q 863094-06-8

NTE scalable

RX(6) RCT Q 863094-06-8

STAGE(1)

SOL 67-56-1 MeOH

CON SUBSTAGE(1) room temperature

SUBSTAGE(2) room temperature

SUBSTAGE(3) room temperature -> 50 deg C

STAGE(2)

RGT L 1333-74-0 H2

CON SUBSTAGE(1) 50 deg C, 30 bar

SUBSTAGE(2) 5 hours, 50 deg C

SUBSTAGE(3) 50 deg C -> room temperature

PRO N 569687-76-9

NTE [Rh((R,R,S,S)-tangphos)(norbornadiene)]BF4 used as catalyst stage 1, stereoselective, high pressure in last stage, autoclave used, ee = 95%, conversion is 100%

RX(30) OF 31 COMPOSED OF RX(5), RX(6), RX(4)

L6 ANSWER 1 OF 6 CASREACT COPYRIGHT 2006 ACS on STN (Continued)

PRO N 569687-76-9

NTE [Rh((R,R,S,S)-tangphos)(norbornadiene)]BF4 used as catalyst stage 1, stereoselective, high pressure in last stage, autoclave used, ee = 95%, conversion is 100%

RX(4) RCT N 569687-76-9

RGT G 1310-73-2 NaOH

PRO K 116539-55-0

SOL 7732-18-5 Water, 75-09-2 CH2Cl2

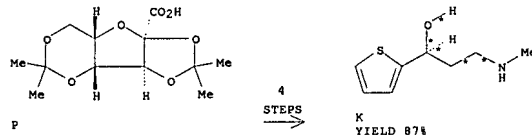
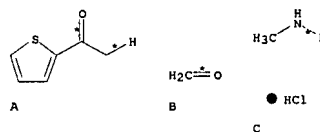
CON SUBSTAGE(1) room temperature

SUBSTAGE(2) 15 minutes, room temperature

NTE incremental addition of reactant

RX(31) OF 31 COMPOSED OF RX(1), RX(5), RX(6), RX(4)

RX(31) A + B + C + P ==> K



RX(1) RCT A 88-15-3, B 50-00-0, C 593-51-1

PRO D 645411-16-1

SOL 64-17-5 EtOH

CON SUBSTAGE(1) 9 hours, 120 - 130 deg C

SUBSTAGE(2) 130 deg C -> 20 deg C

NTE paraformaldehyde used, autoclave used

RX(5) RCT D 645411-16-1

STAGE(1)

RGT G 1310-73-2 NaOH

SOL 7732-18-5 Water, 1634-04-4 t-BuOMe

CON SUBSTAGE(1) room temperature -> 0 deg C

SUBSTAGE(2) 15 minutes, 0 deg C

SUBSTAGE(3) 10 minutes, 0 deg C

STAGE(2)

RGT P 18467-77-1

SOL 1634-04-4 t-BuOMe

L6 ANSWER 1 OF 6 CASREACT COPYRIGHT 2006 ACS on STN (Continued)
CON room temperature

PRO Q 863094-06-8
NTE scalable

RX(6) RCT Q 863094-06-8

STAGE(1)
SOL 67-56-1 MeOH
CON SUBSTAGE(1) room temperature
SUBSTAGE(2) room temperature
SUBSTAGE(3) room temperature -> 50 deg C

STAGE(2)
RGT L 1333-74-0 H2
CON SUBSTAGE(1) 50 deg C, 30 bar
SUBSTAGE(2) 5 hours, 50 deg C
SUBSTAGE(3) 50 deg C -> room temperature

PRO N 569687-76-9
NTE [Rh((R,R,S,S)-tangphos)(norbornadiene)]BF4 used as catalyst stage 1, stereoselective, high pressure in last stage, autoclave used, ee = 95%, conversion is 100%

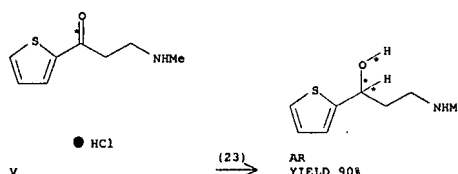
RX(4) RCT N 569687-76-9
RGT G 1310-73-2 NaOH
PRO K 116539-55-0
SOL 7732-18-5 Water, 75-09-2 CH2Cl2
CON SUBSTAGE(1) room temperature
SUBSTAGE(2) 15 minutes, room temperature
NTE incremental addition of reactant

L6 ANSWER 2 OF 6 CASREACT COPYRIGHT 2006 ACS on STN

ACCESSION NUMBER: 142:481782 CASREACT
TITLE: Practical synthesis of enantiopure γ -amino alcohols by rhodium-catalyzed asymmetric hydrogenation of β -secondary-amino ketones
AUTHOR(S): Liu, Duan; Gao, Wenzhong; Wang, Chunjiang; Zhang, Xumu
CORPORATE SOURCE: Department of Chemistry, The Pennsylvania State University, University Park, PA, 16802, USA
SOURCE: Angewandte Chemie, International Edition (2005), 44(11), 1687-1689
CODEN: ACIEF5; ISSN: 1433-7851
PUBLISHER: Wiley-VCH Verlag GmbH & Co. KGaA
DOCUMENT TYPE: Journal
LANGUAGE: English

AB Several β -secondary amino ketone hydrochlorides were hydrogenated with remarkably high enantioselectivities by using a rhodium complex containing P-chiral bisphospholane. These results establish a short and practical means for the synthesis of enantiopure N-monosubstituted γ -amino alcs., which are key intermediates in the synthesis of important antidepressants. For example, the bis(di(methyl)ethyl)tetra(hydro)-1,1'-bi-1H-isophosphindole-rhodium-catalyzed stereoselective hydrogenation of 3-(methylamino)-1-phenyl-1-propanone hydrochloride gave (aS)- α -[2-[(methyl)amino]ethyl]benzenemethanol, which is a synthetic precursor for (yS)-N-methyl- γ -[4-(trifluoromethyl)phenoxy]benzenepropanamine [i.e., (S)-fluoxetine]. The synthesis of (aS)-[2-[(methyl)amino]ethyl]thiophenemethanol, a key synthetic intermediate for (S)-duloxetine, was also reported.

RX(23) OF 74 ...V ==> AR



RX(23) RCT V 645411-16-1

STAGE(1)
RGT Z 16940-66-2 NaBH4
SOL 67-56-1 MeOH
CON SUBSTAGE(1) room temperature
SUBSTAGE(2) 1 hour, room temperature

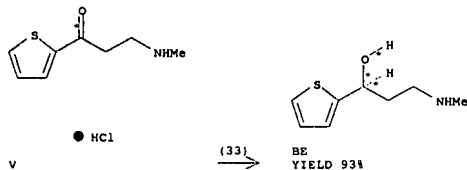
STAGE(2)
RGT AA 12125-02-9 NH4Cl
SOL 7732-18-5 Water
CON room temperature

L6 ANSWER 2 OF 6 CASREACT COPYRIGHT 2006 ACS on STN (Continued)

STAGE(3)
RGT AB 1310-73-2 NaOH
SOL 7732-18-5 Water
CON room temperature, basify

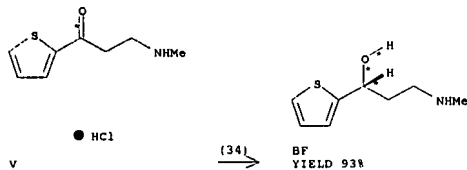
PRO AR 116539-56-1

RX(33) OF 74 ...V ==> BE...



RX(33) RCT V 645411-16-1
RGT AV 584-08-7 K2CO3, AW 1333-74-0 H2
PRO BE 116539-55-0
CAT 851936-69-1 Rhodium(I+), [(2,3,5,6- η)-bicyclo[2.2.1]hepta-2,5-diene][(1S,1'S,2S,2'S)-2,2'-bis(1,1-dimethylethyl)-2,2',3,3'-tetrahydro-1,1'-bi-1H-isophosphindole- κ P2, κ P2']-, (OC-6-11)-hexafluoroantimonate(1-)
SOL 67-56-1 MeOH
CON 12 hours, 50 deg C, 10 bar
NTE stereoselective

RX(34) OF 74 ...V ==> BF



RX(34) RCT V 645411-16-1
RGT AV 584-08-7 K2CO3, AW 1333-74-0 H2
PRO BF 116539-57-2
CAT 850780-91-5 Rhodium(I+), [(2,3,5,6- η)-bicyclo[2.2.1]hepta-2,5-diene][(1R,1'R,2R,2'R)-2,2'-bis(1,1-dimethylethyl)-2,2',3,3'-tetrahydro-1,1'-bi-1H-isophosphindole- κ P2, κ P2']-, (OC-6-11)-hexafluoroantimonate(1-)

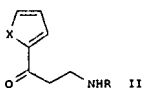
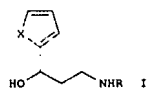
L6 ANSWER 2 OF 6 CASREACT COPYRIGHT 2006 ACS on STN (Continued)

SOL 67-56-1 MeOH
CON 12 hours, 50 deg C, 10 bar
NTE stereoselective
IT 850780-91-5 851936-69-1
RL: CAT (Catalyst use); USES (Uses)
[preparation of chiral γ -amino alc. derivs. by stereoselective hydrogenation of β -secondary amino ketone derivs. using chiral bis(di(methyl)ethyl)tetra(hydro)-1,1'-bi-1H-isophosphindole-rhodium as catalyst]

L6 ANSWER 3 OF 6 CASREACT COPYRIGHT 2006 ACS ON STN

ACCESSION NUMBER: 142:280046 CASREACT
 TITLE: Process for the asymmetric hydrogenation of β -amino ketones using transition metal complexes of chiral bidentate phosphines as catalysts.
 PATENT ASSIGNEE(S): Lonza AG, Switz.
 SOURCE: Eur. Pat. Appl., 15 pp.
 CODEN: EPXXDW
 DOCUMENT TYPE: Patent
 LANGUAGE: English
 FAMILY ACC. NUM. COUNT: 1
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
EP 1510517	A1	20050302	EP 2003-77734	20030901
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, SK				
AU 2004268057	A1	20050310	AU 2004-268057	20040831
WO 2005021527	A2	20050310	WO 2004-EP9690	20040831
WO 2005021527	A3	20050714		
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, GR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW				
RW: BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AE, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
EP 1664014	A2	20060607	EP 2004-764655	20040831
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, FI, RO, CY, TR, BG, CZ, EE, HU, PL, SK				
NO 200600763	A	20060317	NO 2006-763	20060217
PRIORITY APPLN. INFO.:			EP 2003-77734	20030901
			WO 2004-EP9690	20040831
OTHER SOURCE(S):		MARPAT 142:280046		
GI				



AB A process for the preparation of enantiomerically enriched or enantiomerically pure β -amino alcohols. [I: X = S, O; R = (substituted) alkyl, cycloalkyl, aryl, aralkyl] comprises asym. hydrogenation of ketones (II: variables as above) using transition metal complexes of chiral bidentate phosphines as catalysts. Thus, 3-methylamino-1-(thien-2-yl)propan-1-one hydrochloride (preparation given), NaOMe, (S,S)-Me-DuPhos, and [Rh(COD)2]BF₄ were autoclaved

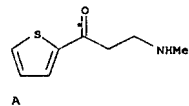
L6 ANSWER 4 OF 6 CASREACT COPYRIGHT 2006 ACS ON STN

ACCESSION NUMBER: 141:348875 CASREACT
 TITLE: L-carnitine dehydrogenase and microorganisms producing L-carnitine dehydrogenase and their use in production of substituted (S)-alkanols
 INVENTOR(S): Althoefer, Henning; Kesseler, Maria
 PATENT ASSIGNEE(S): BASF A.-G., Germany
 SOURCE: Ger. Offen., 41 pp.
 CODEN: GWXXBX
 DOCUMENT TYPE: Patent
 LANGUAGE: German
 FAMILY ACC. NUM. COUNT: 1
 PATENT INFORMATION:

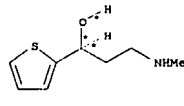
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
DE 10315760	A1	20041021	DE 2003-10315760	20030407
CA 2521218	AA	20041021	CA 2004-2521288	20040406
WO 2004090094	A2	20041021	WO 2004-EP3655	20040406
WO 2004090094	A3	20050317		
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, GR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW				
RW: BW, GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AE, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
EP 1613745	A2	20060111	EP 2004-725924	20040406
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, PL, SK, HR				
CN 1771323	A	20060510	CN 2004-80009243	20040406
JP 2006521800	T2	20060928	JP 2006-505019	20040406
US 2006211099	A1	20060921	US 2005-552218	20051006
PRIORITY APPLN. INFO.:			DE 2003-10315760	20030407
			WO 2004-EP3655	20040406

AB The present invention concerns proteins, which possess an enzymic activity for reduction of substituted alkanones, such as 3-methylamino-1-(2-thienyl)-propan-1-one. Furthermore, the invention concerns nucleic acids which code for these proteins, vectors, and genetically modified microorganisms as well as procedures for the production of substituted (S)-alkanols, e.g., (S)-3-methylamino-1-(2-thienyl)-(S)-propanol. This compound may be used in the synthesis of duloxetine.

RX(1) OF 1 A ==> B



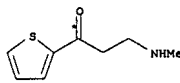
(1)



L6 ANSWER 3 OF 6 CASREACT COPYRIGHT 2006 ACS ON STN (Continued)

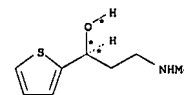
together in MeOH at 30-34° and 30 bar H₂ for 5 h to give 67% (S)-3-methylamino-1-(2-thienyl)-1-propanol in >99% enantiomeric excess.
 REFERENCE COUNT: 6 THERE ARE 6 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

RX(6) OF 7 ...D ==> P



● HCl

(6)



P YIELD 80%

RX(6) RCT D 645411-16-1
 RGT Q 124-41-4 NaOMe, R 1333-74-0 H₂
 PRO P 116539-55-0
 CAT 248244-33-9 5H-Phosphole[3,4-d]-1,3-dioxole, 5,5'-(1,2-phenylene)bis(tetrahydro-2,2,4,6-tetramethyl-, (3aS,3'aS,4S,4'aS,6S,6'aS,6'S,6aS,6'aS)-, 35138-22-8 Rhodium(1+), bis[(1,2,5,6-η)-1,5-cyclooctadiene]-, tetrafluoroborate(1-)
 SOL 67-56-1 MeOH
 CON SUBSTAGE(1) room temperature
 SUBSTAGE(2) 24 hours, 30 - 70 deg C, 30 bar
 NTE high pressure, optimization study, stereoselective
 ST aminoketone asym hydrogenation ruthenium rhodium chiral bidentate phosphine catalyst; aminoalcal chiral prep; aminothiénylpropanone aminofurylpropanone asym hydrogenation; thienylaminoalcal furylaminoalcal chiral prep

L6 ANSWER 4 OF 6 CASREACT COPYRIGHT 2006 ACS ON STN (Continued)

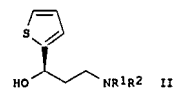
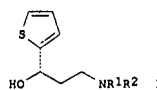
RX(1) RCT A 667465-15-8
 PRO B 116539-55-0
 SOL 7732-18-5 Water
 CON 1 - 23 hour, 30 deg C, pH 7
 NTE biotransformation, described medium, enzymic, stereoselective, L-carnitine dehydrogenase used, carnitine or hydroxycy-CoA-dehydrogenase used
 TI L-carnitine dehydrogenase and microorganisms producing L-carnitine dehydrogenase and their use in production of substituted (S)-alkanols
 ST carnitine dehydrogenase alkanone redn chiral alkanol duloxetine synthesis
 IT Alcohols, preparation
 RL: BPF (Bioindustrial manufacture); BPN (Biosynthetic preparation); BIOL (Biological study); PREP (Preparation)
 (chiral: L-carnitine dehydrogenase and microorganisms producing L-carnitine dehydrogenase and their use in production of substituted (S)-alkanols)
 IT Agrobacterium
 Agrobacterium tumefaciens
 Alcaligenes
 Archaeoglobus
 Archaeoglobus fulgidus
 Enterobacteriaceae
 Mesorhizobium loti
 Molecular cloning
 Nocardiaceae
 Pseudomonadaceae
 Pseudomonas
 Pseudomonas aeruginosa
 Pseudomonas putida
 Rhizobiaceae
 Rhizobium
 Staphylococcus
 Staphylococcus epidermidis
 Streptomyces
 Streptomyces coelicolor
 Streptomycetaceae
 Xanthomonas
 Xanthomonas campestris
 (L-carnitine dehydrogenase and microorganisms producing L-carnitine dehydrogenase and their use in production of substituted (S)-alkanols)
 IT 775366-21-7, Dehydrogenase, carnitine (Alcaligenes)
 775366-22-8 775366-23-9 775366-24-0 775366-25-1 775366-26-2
 775366-27-3 775366-28-4 775366-29-5
 RL: CAT (Catalyst use); PRP (Properties); USES (Uses)
 (amino acid sequence; L-carnitine dehydrogenase and microorganisms producing L-carnitine dehydrogenase and their use in production of substituted (S)-alkanols)
 IT 116539-55-OP
 RL: BPF (Bioindustrial manufacture); BPN (Biosynthetic preparation); BIOL (Biological study); PREP (Preparation)
 (L-carnitine dehydrogenase and microorganisms producing L-carnitine dehydrogenase and their use in production of substituted (S)-alkanols)
 IT 9028-40-4, E.c. 1.1.1.35 9045-45-8, E.c. 1.1.1.108
 RL: CAT (Catalyst use); USES (Uses)
 (L-carnitine dehydrogenase and microorganisms producing L-carnitine dehydrogenase and their use in production of substituted (S)-alkanols)
 IT 667465-15-8

L6 ANSWER 4 OF 6 CASREACT COPYRIGHT 2006 ACS ON STN (Continued)
 RL: RCT (Reactant); RACT (Reactant or reagent)
 (l-carnitine dehydrogenase and microorganisms producing
 l-carnitine dehydrogenase and their use in prodn. of
 substituted (S)-alkanols)
 IT 116539-59-4P, Duloxetine
 RL: SPN (Synthetic preparation); PREP (Preparation)
 (l-carnitine dehydrogenase and microorganisms producing
 l-carnitine dehydrogenase and their use in production of
 substituted (S)-alkanols)
 IT 775366-20-6
 RL: BUU (Biological use, unclassified); PRP (Properties); BIOL (Biological
 study); USES (Uses)
 (nucleotide sequence; l-carnitine dehydrogenase and
 microorganisms producing l-carnitine dehydrogenase and their
 use in production of substituted (S)-alkanols)

L6 ANSWER 5 OF 6 CASREACT COPYRIGHT 2006 ACS ON STN
 ACCESSION NUMBER: 140:321232 CASREACT
 TITLE: Preparation of optically active 3-amino-1-(2-thienyl)-
 1-propanols via reduction of 3-amino-1-(2-thienyl)-1-
 propanones using a hydrogen donor in the presence of a
 metal catalyst, an optically active
 nitrogen-containing ligand and optionally a base.
 INVENTOR(S): Fuchs, Rudolf; Michel, Dominique; Brieden, Walter
 PATENT ASSIGNEE(S): Lonza A.-G., Switz.
 SOURCE: PCT Int. Appl., 25 pp.
 CODEN: PIXXD2
 DOCUMENT TYPE: Patent
 LANGUAGE: English
 FAMILY ACC. NUM. COUNT: 1
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2004031168	A2	20040415	WO 2003-EP11073	20031007
WO 2004031168	A3	20040826		

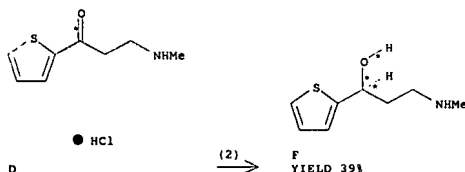
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 CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE,
 GH, GM, GR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK,
 LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MY, NI, NO, NZ,
 OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM,
 TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW
 RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY,
 KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES,
 FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, ES,
 BF, BJ, CF, CG, CI, CM, GN, GG, GW, ML, MR, NE, SN, TD, TG
 AU 20023276066 A1 20040423 AU 2003-276066 20031007
 EP 2002-22540 20021007
 PRIORITY APPLN. INFO.: EP 2003-EP11073 20031007
 OTHER SOURCE(S): MARPAT 140:321232
 GI



AB Title compds. (I, II; R1, R2 = H, alkyl, cycloalkyl, aralkyl, aryl), were
 prepared by reducing the corresponding 3-amino-1-(2-thienyl)-1-propanones
 using a hydrogen donor in the presence of a metal catalyst, an
 optically active N-containing ligand and optionally a base. Thus,
 3-N-methylamino-1-(2-thienyl)-1-propanone hydrochloride (preparation given) and
 NaOH were stirred 1 h in Me2CHOH; a prestirred solution of
 (1S,2R)-cis-1-amino-2-indanol and (p-cymene)ruthenium(II)chloride dimer in
 Me2CHOH was added followed by stirring for 4 h at 20° to give 39%
 (S)-N-methylamino-1-(2-thienyl)-1-propanol in 70% enantiomeric excess.

RX(2) OF 5 ...D ==> F

L6 ANSWER 5 OF 6 CASREACT COPYRIGHT 2006 ACS ON STN (Continued)



RX(2)

STAGE(1)
 CAT 126456-43-7 1H-Inden-2-ol, 1-amino-2,3-dihydro-, (1S,2R)-,
 52462-29-0 Ruthenium, di-μ-chlorodichlorobis[(1,2,3,4,5,
 6-n)-1-methyl-4-(1-methylethyl)benzene]di-
 SOL 67-63-0 Me2CHOH
 CON SUBSTAGE(1) 20 minutes, 85 deg C
 SUBSTAGE(2) 85 deg C -> 20 deg C

STAGE(2)
 RCT D 645411-16-1
 RGT G 1310-73-2 NaOH
 SOL 67-63-0 Me2CHOH
 CON SUBSTAGE(1) 1 hour, 20 deg C
 SUBSTAGE(2) 20 deg C
 SUBSTAGE(3) 4 hours, 20 deg C

PRO F 116539-55-0
 NTE stereoselective

TI Preparation of optically active 3-amino-1-(2-thienyl)-1-propanols via
 reduction of 3-amino-1-(2-thienyl)-1-propanones using a hydrogen donor in
 the presence of a metal catalyst, an optically active
 nitrogen-containing ligand and optionally a base.
 AB Title compds. (I, II; R1, R2 = H, alkyl, cycloalkyl, aralkyl, aryl), were
 prepared by reducing the corresponding 3-amino-1-(2-thienyl)-1-propanones
 using a hydrogen donor in the presence of a metal catalyst, an
 optically active N-containing ligand and optionally a base. Thus,
 3-N-methylamino-1-(2-thienyl)-1-propanone hydrochloride (preparation given) and
 NaOH were stirred 1 h in Me2CHOH; a prestirred solution of
 (1S,2R)-cis-1-amino-2-indanol and (p-cymene)ruthenium(II)chloride dimer in
 Me2CHOH was added followed by stirring for 4 h at 20° to give 39%
 (S)-N-methylamino-1-(2-thienyl)-1-propanol in 70% enantiomeric excess.

IT Reduction catalysts
 (preparation of optically active aminothiethylpropanols via reduction of
 aminothiethylpropanones using a hydrogen donor in the presence of a
 metal catalyst, an optically active N-containing ligand and a
 base)

IT Reduction
 (stereoselective; preparation of optically active aminothiethylpropanols via
 reduction of aminothiethylpropanones using a hydrogen donor in the presence
 of a metal catalyst, an optically active N-containing ligand and
 a base)

IT 7439-88-5D, Iridium, organometallic complexes 7440-16-6D, Rhodium,
 organometallic complexes 52462-29-0, (p-cymene)ruthenium(II)chloride
 dimer 126456-43-7

L6 ANSWER 5 OF 6 CASREACT COPYRIGHT 2006 ACS ON STN (Continued)

RL: CAT (Catalyst use); USES (Uses)
 (prepn. of optically active aminothiethylpropanols via redn. of
 aminothiethylpropanones using a hydrogen donor in the presence of a
 metal catalyst, an optically active N-contg. ligand and a
 base)

IT 116539-55-0P 132335-44-5P 625853-20-5P
 RL: INF (Industrial manufacture); SPN (Synthetic preparation); PREP
 (Preparation)
 (preparation of optically active aminothiethylpropanols via reduction of
 aminothiethylpropanones using a hydrogen donor in the presence of a
 metal catalyst, an optically active N-containing ligand and a
 base)

IT 64-17-5, Ethanol, uses
 RL: NUU (Other use, unclassified); USES (Uses)
 (preparation of optically active aminothiethylpropanols via reduction of
 aminothiethylpropanones using a hydrogen donor in the presence of a
 metal catalyst, an optically active N-containing ligand and a
 base)

IT 67-63-0, Isopropanol, reactions
 RL: NUU (Other use, unclassified); RGT (Reagent); RACT (Reactant or
 reagent); USES (Uses)
 (preparation of optically active aminothiethylpropanols via reduction of
 aminothiethylpropanones using a hydrogen donor in the presence of a
 metal catalyst, an optically active N-containing ligand and a
 base)

IT 88-15-3, 2-Acetylthiophene 593-51-1, Methylamine hydrochloride
 13196-35-5 18467-77-1, (-)-2,3,4,6-Di-O-isopropylidene-2-keto-L-gulonic
 acid 30525-89-4, Paraformaldehyde 114559-95-4, (+)-2,3,4,6-Di-O-
 isopropylidene-2-keto-D-gulonic acid 132335-48-9
 RL: RCT (Reactant); RACT (Reactant or reagent)

(preparation of optically active aminothiethylpropanols via reduction of
 aminothiethylpropanones using a hydrogen donor in the presence of a
 metal catalyst, an optically active N-containing ligand and a
 base)

IT 569687-76-9P 645411-16-1P, 3-N-Methylamino-1-(2-thienyl)-1-propanone
 hydrochloride 679405-09-5P 679405-10-8P 679405-11-9P 679405-12-0P
 RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT
 (Reactant or reagent)

(preparation of optically active aminothiethylpropanols via reduction of
 aminothiethylpropanones using a hydrogen donor in the presence of a
 metal catalyst, an optically active N-containing ligand and a
 base)

IT 1310-58-3, Potassium hydroxide, reactions 1310-73-2, Sodium hydroxide,
 reactions
 RL: RGT (Reagent); RACT (Reactant or reagent)
 (preparation of optically active aminothiethylpropanols via reduction of
 aminothiethylpropanones using a hydrogen donor in the presence of a
 metal catalyst, an optically active N-containing ligand and a
 base)

10/542,003

L6 ANSWER 6 OF 6 CASREACT COPYRIGHT 2006 ACS on STN (Continued)
IT 114133-37-8P, (S)-3-(Methylamino)-1-phenyl-1-propanol 116539-55-0P,
(S)-3-(Methylamino)-1-(2-thienyl)-1-propanol
RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation amino alcs. via the enantioselective hydrogenation of
amino ketones with chiral diphosphine ligands)

10/5/2006

10/542,003

=> s 14 not 15

L5 MAY NOT BE USED HERE

The L-number entered was not created by a STRUCTURE or SCREEN command.

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(FILE 'HOME' ENTERED AT 14:28:45 ON 05 OCT 2006)

FILE 'CASREACT' ENTERED AT 14:29:17 ON 05 OCT 2006

L1 STRUCTURE UPLOADED

L2 8 S L1 FUL

L3 6 S L2 AND (ENZYME OR MICROBIAL OR DEHYDROGENASE OR CATALYST OR E

FILE 'CASREACT' ENTERED AT 14:32:46 ON 05 OCT 2006

L4 STRUCTURE UPLOADED

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L6 6 S L5 AND (ENZYME OR MICROBIAL OR DEHYDROGENASE OR ENANTIOSELECT

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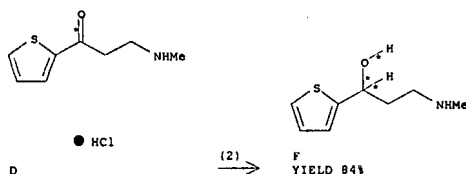
L7 2 L5 NOT L6

=> d ibib hit 1-2

L7 ANSWER 1 OF 2 CASREACT COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 140:93915 CASREACT
TITLE: Process for the preparation of optically active
3-N-methylamino-1-(2-thienyl)-1-propanol
INVENTOR(S): Michel, Dominique
PATENT ASSIGNEE(S): Lonza A.-G., Switz.
SOURCE: PCT Int. Appl., 34 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
NO 2004005307	A1	20040115	WO 2003-EP7312	20030708
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW				
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
AU 2003253036	A1	20040123	AU 2003-253036	20030708
PRIORITY APPLN. INFO.:			EP 2002-15161	20020709
			WO 2003-EP7312	20030708
OTHER SOURCE(S):	MARPAT 140:93915			
REFERENCE COUNT:	4	THERE ARE 4 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT		

RX(2) OF 4 ...D ==> F



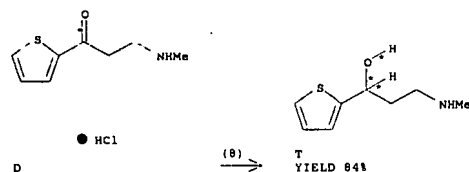
RX(2) RCT D 645411-16-1

STAGE(1)
RGT G 1310-73-2 NaOH, H 16940-66-2 NaBH4
SOL 64-17-5 EtOH
CON SUBSTAGE(1) 5 minutes, 4 deg C
SUBSTAGE(2) 30 minutes, 4 deg C

L7 ANSWER 2 OF 2 CASREACT COPYRIGHT 2006 ACS on STN
ACCESSION NUMBER: 140:93914 CASREACT
TITLE: Process for the preparation of N-monosubstituted
β-amino alcohols
INVENTOR(S): Michel, Dominique
PATENT ASSIGNEE(S): Lonza A.-G., Switz.
SOURCE: PCT Int. Appl., 28 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2004005239	A1	20040115	WO 2003-EP7411	20030709
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW				
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
CA 2491472	AA	20040115	CA 2003-2491472	20030709
AU 2003250924	A1	20040123	AU 2003-250924	20030709
BR 2003012651	A	20050426	BR 2003-12651	20030709
EP 1539673	A1	20050615	EP 2003-762669	20030709
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, SK				
CN 1665773	A	20050907	CN 2003-816223	20030709
JP 2005332383	T2	20051027	JP 2004-518758	20030709
NO 2005000079	A	20050311	NO 2005-79	20050106
US 2005256318	A1	20051117	US 2005-520362	20050418
PRIORITY APPLN. INFO.:			EP 2002-15229	20020709
			WO 2003-EP7411	20030709
OTHER SOURCE(S):	MARPAT 140:93914			
REFERENCE COUNT:	15	THERE ARE 15 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT		

RX(8) OF 11 ...D ==> T



RX(8) RCT D 645411-16-1

L7 ANSWER 1 OF 2 CASREACT COPYRIGHT 2006 ACS on STN (Continued)
SUBSTAGE(3) 4 hours, 4 deg C

STAGE(2)
SOL 67-64-1 Me2CO
CON SUBSTAGE(1) 5 minutes
SUBSTAGE(2) 10 minutes

STAGE(3)
SOL 7732-18-5 Water

PRO F 116539-56-1

L7 ANSWER 2 OF 2 CASREACT COPYRIGHT 2006 ACS on STN (Continued)
STAGE(1)
RGT U 16940-66-2 NaBH4, V 1310-73-2 NaOH
SOL 7732-18-5 Water, 64-17-5 EtOH
CON SUBSTAGE(1) 5 minutes
SUBSTAGE(2) 30 minutes
SUBSTAGE(3) 4 hours

STAGE(2)
SOL 67-64-1 Me2CO
CON SUBSTAGE(1) 5 minutes
SUBSTAGE(2) 10 minutes

STAGE(3)
SOL 7732-18-5 Water

PRO T 116539-56-1